BEILSTEIN SYMPOSIUM

Defect-mediated engineering of nanomaterials for energy and quantum applications

Beilstein Nanotechnology Symposium 2025

May 13–15, 2025
Hotel Jagdschloss Niederwald
Rüdesheim (Rhein), Germany

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Our two diamond open access journals, the *Beilstein Journal of Organic Chemistry* and the *Beilstein Journal of Nanotechnology*, which we fully fund, have no fees for authors or readers. Both journals are produced and managed by the Beilstein Editorial Office team, who work together with a global scientific network of experts that are responsible for the peer review, ensuring high quality science is published. In 2015, the Beilstein Journals were awarded the DOAJ Seal which recognizes the exceptionally high level of publishing standards and best practices adhering to these journals. Both journals publish thematic issues on subjects of high contemporary interest; these are often edited by guest editors, further expanding our network and outreach.

Launched in April 2019, a new addition to our publishing platform is the Beilstein Archives. This is the preprint server for the Beilstein journals. During the manuscript submission process, authors have the option to request that the manuscript is posted as a preprint, which is the version of the manuscript before peer review. Our preprints are posted on average within two days, allowing authors to rapidly disseminate their research results and ensuring that they claim priority for their work. Currently, over 30% of our authors select the preprint option.

The Beilstein-Institut runs two data standards projects: STRENDA which is concerned with the reporting of enzymology data and MIRAGE which is working on guidelines for the reporting of glycomics experimental results. Both of which are now widely accepted and acknowledged by the scientific community.

The direct interaction and the exchange of thoughts and ideas between scientists are supported by a program of regularly hosted symposia. These international meetings are organized by the Beilstein-Institut and cover a variety of topics ranging from organic chemistry and biochemistry to nanotechnology and open science as well as interdisciplinary meetings on contemporary topics.

The Beilstein-Institut has been hosting symposia since 1988. Each meeting is always a unique event with an open result: The Beilstein-Institut provides the framework and the lively and intense exchange of thoughts and ideas of the participants turn it into a memorable and lasting experience. The number of participants is usually limited to around 50 and the program is designed specifically to allow sufficient time for discussions. In some ways the talks can be seen as providing a catalyst for these discussions which often go on into the night and have led to subsequent cooperation projects. The resulting exchange between researchers, at all stages of their careers, is the underlying goal of the meeting and gives the Beilstein Symposium their unique character.

Regularly updated information about our symposia is available at
www.beilstein-symposia.org.

Book of Abstracts

Table of Contents

Overview

Defects, which are ubiquitous in crystalline solids at finite temperatures due to the second law of thermodynamics, are also present in two-dimensional (2D) systems, an important class of materials which have recently received enormous amount of attention. Moreover, many 2D materials are synthetic, so that defect concentration in them can be well above the equilibrium value. 2D materials consist of essentially surface only, so that defects can easily be formed due to the interaction with the environment, e.g., because of oxidation. The imperfections have a strong influence on the electronic, optical, thermal, and mechanical properties of 2D materials, normally deteriorating their characteristics, but can also be beneficial, e.g., in the context of doping or single-photon quantum emitters. The reduced dimensionality of 2D materials strongly enhances the role of defects (detrimental or beneficial), and many concepts of the physics of defects in bulk systems are not applicable for 2D materials or require substantial modifications.

This symposium will bring together scientists focused on the physics of defects in 2D materials to discuss recent progress and challenges in the field, including "state of the art" in theory and characterization techniques.

The symposium will cover, but is not limited to the following themes:

/ Defects in 2D materials for quantum technologies

/ Characterization of defects in 2D materials

/ Doping of 2D materials

/ First-principles modeling of native defects and impurities in 2D materials

/ Production of defects in 2D materials under ion-irradiation

/ Electron-beam-mediated engineering of 2D materials through controllable introduction of defects

The Beilstein Symposia address contemporary issues in chemistry and neighboring sciences by emphasizing interdisciplinarity. Scientists from a wide range of areas – often outside chemistry – are invited to present (provoking) aspects of their work for “out of the box” discussion with the aim not only to advance science, but also to enhance interdisciplinary communication.

We are looking toward committed discussions about the latest results, approaches and methodologies presented in the various experimental, theoretic and informatics research fields. Enjoy the symposium!

Scientific Committee

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Presentations of Posters

Poster exhibition

On Tuesday, we will have a dedicated poster session and three flash talk sessions spread throughout the day.

Location of the posters

The poster exhibition will be placed in the coffee room which is close to the conference room. Your poster board will be marked with your poster number which is the same in the abstract book.

Poster mounting

Please mount your poster before the session. You can start hanging them from Monday, May 12, after 5 PM. Your poster will be on display throughout the symposium. You are asked to remove all poster materials from the board at the end of the meeting.

Poster material

The size of your poster board is 120 x 90 cm (height x width). Hanging material for the poster boards will be provided on-site.

Presentations

The oral poster presentations will take place as indicated in the scientific program. The presentations should not exceed 5 min. You will have 1 min in addition for questions.

Please make sure that you have delivered your final presentation to the organizers in time.

We will have an LCD projector connected to a Windows PC available.

Liability and Insurance

The Beilstein-Institut will not be liable for any accident, theft or damage to property, nor for any delays or modification in the program due to unforeseen circumstances.

Participants and accompanying persons are advised to arrange personal travel and health insurance.

Scientific Program

Monday, 12th May

19:00 Welcome Reception

19:30 Dinner

Tuesday, 13th May

09:00	Welcome And Opening	Beilstein-Institut
	Session Chair: Chris Ewels	
09:20	Point And Line Defects In Monolayer MoS_2	Thomas Michely
10:00	Data-Driven Discovery Of Novel Point Defects For Quantum Technology	Kristian Thygesen
10:40	Poster Lightning Talks #1 (Posters 1-4)	
11:00	*Coffee Break*	
	Session Chair: Thomas Michely	
11:20	Chirality Switching In 1T -TaS_2 Induced By Highly Charged Ion Irradiation	Richard Wilhelm
12:00	Defect-Engineering Of Devices Based On 2D Materials	Marika Schleberger
12:40	Poster Lightning Talks #2 (Posters 5-8)	
13:00	*Lunch*	
	Session Chair: Richard Wilhelm	
14:30	Optical Properties Of Atomistic Quantum Emitters In 2D Materials	Alexander Holleitner
15:10	The Influence Of Dopants And Substrates On Defects In 2D Semiconductors	Joshua A. Robinson
15:50	Poster Lightning Talks #3 (Posters 9-13)	
16:10	*Conference Photo And Coffee Break*	
	Session Chair: Jani Kotakoski	
16:40	Defect Engineering For Materials Design: Complexity And Challenges	Yun Liu
17:20	The Role Of Atomic Defects In Phase Engeneering Of 2D Van-Der-Waals Structures	Ute Kaiser
18:00	Poster Session	
19:30	*Dinner*	

Wednesday, 14th May

09:00	Opening	
	Session Chair: Bruno Schuler	
09:05	Stem/Eels Analysis Of Low Dimensional Structures With Defects	Kazu Suenaga
09:45	Topological Engineering Of Magnetism With Edge Defects In Graphene Nanoribbons	Steven G. Louie
10:25	Individual S Vacancies And Their Role In Anchoring Of Organic Molecules On Monolayers Of MoS_2	Katharina Franke
11:05	*Coffee Break*	
	Session Chair: Kristian Thygesen	
11:40	Light Emission And Excitation Of Single Atomic Defects In 2D Semiconductors	Bruno Schuler
12:20	Optical Properties Of Defects In 2D Materials	Janina Maultzsch
13:00	*Lunch*	
14:00-17:30	*Excursion*	
19:30	*Dinner*	

Thursday, 15th May

09:00	Opening	
	Session Chair: Hannu-Pekka Komsa	
09:05	Structure, Chemistry And Electrostatic Potential In Defective TMDs Probed By 4D-Stem	Hanako Okuno
09:45	Atomically-Precise Tailored Structures Within 2D Materials	Jani Kotakoski
10:25	Tip-Enhanced Raman Spectroscopy Of Two-Dimensional Systems	Ado Jório
11:05	*Coffee Break*	
	Session Chair: Matthias Batzill	
11:40	Defect Mediated Growth Of 2D Metallenes	Harriet Åhlgren
12:20	Role Of Defects In Oxidation Of WS_2 Surfaces And Interfaces	Alexander Shluger
13:00	*Lunch*	
	Session Chair: Ado Jório	
14:30	Modifications Of Transition Metal Dichalcogenides By Incorporation Of Excess Transition Metals	Matthias Batzill
15:10	Screening Of Material Defects Using Universal Machine-Learning Interatomic Potentials	Hannu-Pekka Komsa
15:50	*Coffee Break*	
	Session Chair: Arkady Krasheninnikov	
16:20	Creation And Characterization Of Nanopores In Hexagonal Boron Nitride Via Aberration-Corrected Scanning Transmission Electron Microscopy	Marija Drndić
17:00	Computer Modelling Of Dislocations In Layered Materials	Chris Ewels, CNRS Nantes
17:40	Closing Remarks	Beilstein-Institut
19:30	*Dinner*	

List of Posters

The poster presentation includes a short (5 min) oral presentation on Tuesday, 13th May, and the poster sessions. The posters will be displayed from Tuesday, 13th May, to Thursday, 15th May.

#1	Room Temperature Gas Sensing With Hierarchical Bi-Doped Sb_2WO_6 Microspheres: Effect Of Oxygen Vacancies	Zichen Zheng
#2	Defect-Engineering Hexagonal Boron Nitride Using Low-Energy Ar^+ Irradiation	Manuel Längle
#3	Defect Engineering In MoS_2 Nanomaterials Via Low-Energy Ion Implantation For Next-Generation 2D Functional Devices	Nawaz Rabia
#4	Spectrally Resolved Far-Field Emission Pattern Of Single Sulfur Vacancies Acting As Single Photon Emitters In MoS_2	Alexander Musta
#5	Revealing The Atomistic Structure Of Carbon Nanomembranes: Molecular Dynamics Simulations And Experiments With Highly Charged Ions	Vukovic Filip
#6	Atomic Manipulation Approach Towards Defect Engineering In Two-Dimensional Materials	Daniel Jansen
#7	Nanoscale Engineering Of Defects In Hexagonal Boron Nitride With An Electron Beam And Its Applications From Quantum Technology To Nanofluidics	Rachael Keneipp
#8	Nanostructuring Of 2D Materials Using Slow Highly Charged Ions	Anna Niggas
#9	Correlated Optical & Structural Characterization Of HBN	Pia Bhatia
#10	Controlled Substitutional Doping Of MoS2 For Gas Sensing Applications	David Lamprecht
#11	2D Passivated Dimethyl Sulfoxide (Dmso) Free Tin Halide Perovskite Over 10%	Muhammad Okash Ur Rehman
#12	Mycosynthesis Of Silver Nanoparticles For Energy Applications	Jayaraju Nadimikeri
#13	Defect-Induced Modulation Of The Electronic And Magnetic Properties In CrSBr Monolayers	Mahdi Ghorbani-Asl

Abstracts

Tuesday

09:20

Point and Line Defects in Monolayer MoS_2

Thomas Michely

University of Cologne,
Institute of Physics II,
Cologne, Germany

Depending on the preparation conditions, monolayers of transition metal dichalcogenides present a variety of point defects. In molecular beam epitaxy (MBE) of transition metal dichalcogenides on graphene under ultrahigh vacuum conditions point defects a virtually absent. Therefore, we developed a new method to create point defects in a controlled way using deposited adatoms and the tip of a scanning tunneling microscopy. The thorough investigation of thereby created S-vacancies in MoS_2 reveals that upon charging the vacancy states within the band gap of MoS_2 experience two different Jahn-Teller distortions [1].

Contrary to point defects, line defects in the form of mirror twin boundaries (MTBs) are frequent in MBE grown single layers of MoS_2 and emerge from coalescence of MoS_2 islands. They form cavities for electrons and can be used as a laboratory for one dimensional (1D) physics. The 1D band linked to the MTB originates from the necessity to compensate polarization charge arising at discontinuities in the polar MoS2. Using scanning tunneling spectroscopy, we determine the polarization charge to be 2/3 of an electron per unit cell along the boundary in full agreement with theoretical predictions [2,3]. While mirror twin boundaries are obstacles for transport normal to them, they can successfully be applied as ultimately thin gates in field effect transistors [4,5].

Through the excellent insulation from the environment and their 1D character, electronic correlations in the wires are strong. Therefore, low-energy electronic excitations are expected to be bosonic collective modes, which fractionalize into independent spin- and charge-density waves. Indeed, measuring the single particle density by scanning tunneling microscopy a Tomonaga-Luttinger liquid is documented in finite length boundaries [6]. Moreover, mirror twin boundaries can be used to construct a new type of Kondo system, for which the entire

spectral function is resolved, including the impurity levels underlying the resonance. Using this information, with the help of numerical renormalization group calculations one is able to test the predictive power of the Anderson model with high accuracy [7,8].

Contributions to this work by Theo A. Costi, Achim Rosch, Hannu-Pekka Komsa, Arkady V. Krasheninnikov, Nicolae Atodiresei, Fabian Portner, Philipp S. Weiß, Wouter Jolie, Clifford Murray, Joshua Hall, Carsten Busse, Camiel van Efferen, Jeison A. Fischer, Mahasweta Bagchi, Tfyeche Y. Tounsi, Affan Safeer, and Daniel Jansen are gratefully acknowledged.

References

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[2] *Band bending and valence band quantization at line defects in MoS_2*, C. Murray et al., Nano Lett. 14 (2020) 9176.
[3] *Emergence of one-dimensional wires of free carriers in transition-metal-dichalcogenide nanostructures*, M. Gibertini & N. Marzari, Nano Lett. 15(2015) 6229.
[4] *Integrated 1D epitaxial mirror twin boundaries for ultrascaled 2D MoS_2 field-effect transistors*, H. Ahn et al., Nat. Nanotechnol. 19 (2024) 955.
[5] *1D metals for 2D electronics*, W. Jolie & T. Michely, Nat. Nanotechnol. 19 (2024) 883.
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[7] *Modulated Kondo screening along magnetic mirror twin boundaries in monolayer MoS_2*, C. van Efferen et al., Nat. Phys. 20 (2024) 82.
[8] *Spin-polarized scanning tunneling microscopy measurements of an Anderson impurity*, M. Bagchi et al., Phys. Rev. Lett. 133 (2024) 246701.

Tuesday

10:00

Data-driven Discovery of Novel Point Defects for Quantum Technology

Kristian S. Thygesen

Technical University of Denmark,
Physics,
Lyngby, Denmark

I will present our data-driven strategies to the *in-silico* design of novel point defects for quantum technology applications. Using the *GPAW* electronic structure code, we perform high-throughput density functional theory (DFT) calculations to screen thousands of point defects in bulk and two-dimensional host materials. The elementary physical properties comprising the key design parameters are the magnetic states of the defect (including zero-field splittings for high-spin states), the optical excitation energy (zero phonon line), and the photoluminescence (PL) line shape. We use the Python workflow framework *TaskBlaster* to compose, manage, and execute the computational workflows, which can be complex and involve dynamic branching and inter-dependent tasks. By integrating the DFT calculations with machine learning technologies, we achieve an order of magnitude speed-up of the otherwise costly calculation of PL spectra.

In addition, I will introduce a unique suite of open computational databases on 2D materials, including the C2DB (monolayers), the BiDB (homobilayers), the HetDB (heterobilayers), and the QPOD (point defects), and discuss our ongoing efforts to integrate these computational databases with experimental data.

If time allows, I will also present a recent study of room temperature quantum emitters in van der Waals MoO_3 flakes.

Tuesday

11:20

Chirality Switching in 1T -TaS2 Induced by Highly Charged ion Irradiation

R.A. Wilhelm[1], A. Niggas[1], J. Buck[2], D. Thima[1], V. Vojtech[1], F. Vukovic[1], M. Werl[1], K. Rossnagel[2]

[1]TU Wien, Institute of Applied Physics, Vienna, Austria

[2]Deutsches Elektronen-Synchrotron DESY, Ruprecht Haensel Laboratory, Hamburg, Germany

It was recently shown that slow highly charged ions (HCIs) can perforate single two-dimensional layers in a van-der-Waals stack [1]. The ultimate surface sensitivity in atomic-scale defect formation of this class of ions stems from the very localized, highly efficient interaction of the HCI with the electronic sub-system of a material [2]. Strong electronic excitations then couple to lattice atomic motion, causing formation of defects or pores.

As the surface electronic state is the determining factor for the susceptibility for nanostructure formation from strong electronic excitations in general, we use *1T*-TaS_2, a prototypical charge-density-wave phase material. *1T*-TaS_2 undergoes a series of phase transitions from a metallic state to a Mott insulating state and provides therefore a platform to test HCI-induced defect formation scenarios with the same material, only varying the electronic properties.

We monitor ion-induced defect formation *in operando* by angle-resolved photoelectron spectroscopy (ARPES) using 400 eV soft X-rays with fixed helicity, provided from the PETRA III synchrotron at DESY. Figure 1 (see printed version) shows ARPES maps at specific energies before and after a total Xe^{8+} ion fluence of $9x10^{11}/cm^2$ at 22.5 keV kinetic energy was applied to bulk *1T*-TaS_2 at 50K (commensurate charge-density-wave Mott insulator phase). One can clearly see that the ARPES map changes the intensity distribution and the difference plot in (c) and (g) indicate that the intensity redistributes according to a mirroring across the Γ-M direction.

In this contribution I will discuss defect mechanisms driving a surface chirality switch from HCIs at low ion fluencies, where surface amorphization is still negligible.

References

[1] Schwestka, J. *et al.* Atomic-Scale Carving of Nanopores into a van der Waals Heterostructure with Slow Highly Charged Ions. *ACS Nano* **14**, 10536–10543 (2020).

[2] Wilhelm, R. A. *et al.* Interatomic Coulombic Decay: The Mechanism for Rapid Deexcitation of Hollow Atoms. *Physical Review Letters* **119**, 103401 (2017).

Tuesday

12:00

Defect-engineering of Devices Based on 2D Materials

Stephan Sleziona, Leon Daniel, Jennifer Schmeink, M. Schleberger

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Faculty of Physics,
Duisburg, Germany

In modern electronics, the active material is only a few atoms thick, so defects play an important role in device properties. For example, in field-effect transistors (FET) using silicon as the channel material, the mobility typically decreases when the channel dimensions become too small due to a high density of dangling bonds on the silicon surface. In the search for alternative materials, two-dimensional (2D) materials have become increasingly attractive. Because of their van-der-Waals structure they can be fabricated with a uniform thickness of only three atomic layers, and ideally free of strain and dangling bonds.

The transition metal dichalcogenides (TMDCs) such as MoS_2 and WS_2 are particularly attractive for applications, as they become direct semiconductors in the monolayer form with a band gap in the visible range, and numerous optoelectronic applications have been demonstrated. However, their performance is strongly controlled by defects. Depending on the application these can be either beneficial or detrimental. This is a challenge, but can also be an opportunity to develop optimized or even novel devices as well as defect engineering strategies.

Tuesday

14:30

Optical Properties of Atomistic Quantum Emitters in 2D Materials

Alexander W. Holleitner

Walter Schottky Institut and Physics Department,
TU Munich,
Munich, Germany

We highlight recent advances in the controlled creation of single-photon emitters in van der Waals materials and in the understanding of their atomistic origin (Figure 1 (see printed version) and Ref. [1]). A particular emphasis will be put on the optical properties of quantum emitters in MoS_2 as produced by the help of a focused beam of helium-ions. Moreover, we introduce a back-focal plane spectroscopy to explore the underlying level structure of the quantum emitters, and in the case of in MoS_2, compare the obtained data to an analytical model as well as to ab initio results as computed from GW and Bethe-Salpeter equation approximations [2].

We acknowledge funding from the DFG-excellence cluster Munich Center of Quantum Science and Technology (MCQST).

References

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[2] Spectrally resolved far-field emission pattern of single photon emitters in MoS_2, K Barthelmi, T. Amit, L. Sigl, M. Troue, T. Klokkers, A. Herrmann, T. Taniguchi, K. Watanabe, J.J. Finley, C. Kastl, S. Refaely-Abramson, A.W. Holleitner, Phys. Rev. Mat. 9, 016201 (2025).

Tuesday

14:25

The Influence of Dopants and Substrates on Defects in 2D Semiconductors

Joshua A. Robinson

Pennsylvania State University,
Materials Science and Engineering,
University Park, USA

The last decade has seen an exponential growth in the science and technology of two-dimensional materials. Beyond graphene, there is a huge variety of layered materials that range in properties from insulating to superconducting. Furthermore, defects and substrates can have a dramatic impact on the growth and propoerties of these systems, as they are all surface. In this talk, I will discuss recent breakthroughs in two-dimensional atomic layer synthesis, properties, and integration toward advancing our understanding of the role defects (dopants, vacancies) play in the synthesis of 2D materials. This includes formation of novel 2D heterostructures and the realization of unique 2D allotropes of 3D materials (e.g. 2D metals, nitride, oxides) based on a novel synthesis method, dubbed confinement heteroepitaxy (CHet). By shrinking traditional metals to atomically thin structures, we find that their properties are completely different than their bulk counterparts, lending themselves to unique quantum and optical applications not possible before.

References

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[5] Nature Materials 15, 1166–1171

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[7] *Nano Lett.* 2022, 22, 19, 7841–7847

[8] Advanced Funct. Materials, 2005977

[9] Advanced Electronic Materials 11 (3), 2400403

[10] Carbon 227, 119260

Tuesday

16:40

Defect Engineering for Materials Design: Complexity and Challenges

Yun Liu

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Research School of Chemistry,
Canberra, Australia

Doping and substitution in solids are powerful strategies for tailoring materials to enhance performance or to create entirely new materials with novel functionalities. These approaches contribute to the vibrancy and diversity of materials research—but also to its inherent complexity. This complexity arises because the average structure revealed by x-ray crystallography often fails to capture the true positions of atoms in materials. Instead, local structures across various length scales must be considered. Defects introduced through doping or substitution can reside in different local chemical and structural environments, leading to diverse and sometimes unexpected impacts on material properties. Moreover, the local environment itself may adjust to accommodate specific doping or substitution atoms, further complicating scenarios. As a result, inconsistencies often arise between observed properties and predicted trends. Therefore, to understand the multiscale structure and construct precise structural models becomes highly nontrivial in many strongly correlated solid-state material systems for defect design.

In this presentation, I will share our research and discuss challenges in materials characterisation and design. This includes the distinction between average and local structures in solids; the local consequences of doping/substitution and their impact on physical properties; structural complexity and defect engineering in 2D materials; and nano-scale interactions and emerging defect engineering strategies; and a potential approach that could overcome the limitations of conventional crystallography. Together, these indicate that to rationally design and fully understand nanomaterials, including 2D materials, it is essential to construct precise structural and defect models, beyond its average structure level for better understanding and designing materials and harnessing their application potentials.

Tuesday

17:20

The Role of Atomic Defects in Phase Engeneering of 2D Van-der-Waals Structures

Ute Kaiser

University of Ulm,
Institute for Quantum Optics,
Ulm, Germany

We show that targeted energy input from an electron beam in a transmission electron microscope (TEM), often combined with concurrent heating in a MEMS holder, drives atomic defect formation and phase transitions across four classes of low-dimensional materials: (1) few-layer transition metal phosphorus trichalcogenides (TMPTs), (2) graphene sandwich structures encapsulating either lithium droplets (2a) or a benzenehexathiol-based two-dimensional conjugated metal-organic framework (2b), (3) platinum nanocrystals on graphene, and (4) noble metals confined within carbon nanotubes.

In (1), controlled heating around 600 °C induces phase transitions to MnS, MnSe, and NiSe, with ab initio calculations predicting orientation- and thickness-dependent magnetic properties. In (2a), graphene vacancies nucleate polycrystalline lithium growth during lithiation, while interstitial oxygen inhibits delithiation via lithium oxide formation. Despite high beam resistance, Cu_3(BHT) (2b) transforms thermally into a crystalline CuS phase between 480 °C and 620 °C as well as under high electron flux. For (3), we resolve the solid–liquid phase transition of Pt nanoclusters and identify a mechanism where stationary Pt atoms corral molten nanodroplets, halting crystallization. Finally, in (4), we reveal contrasting bonding behaviors of Re and Kr atoms within fullerenes inside carbon nanotubes, driven by differences in electronic structure and confinement.

These findings are enabled by the Cc/Cs-corrected SALVE (Sub-Ångström Low-Voltage TEM) platform, highlighting its potential for atomic-scale in situ phase engineering.

Wednesday

09:05

STEM/EELS Analysis of Low Dimensional Structures with Defects

Kazu Suenaga

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The Institute for Scientific and Industrial Research (SANKEN),
Iberaki, Japan

Properties of low-dimensional materials are largely influenced by its structural imperfections, such as defects, impurities, edges or boundaries. Hence, analytical technique at single atom level is becoming crucial to fully understand the physical/chemical performance of nano-devices. In my presentation, single atom spectroscopy by means of electron energy-loss spectroscopy (EELS) will be shown to discriminate individual atoms in low-dimensional materials at their interrupted periodicities. It is emphasized here that information of the bonding/electronic states has become accessible for single atoms through the EELS fine-structure analysis [1, 2, 3] as well as the spin state [4]. Large variations of local electronic properties of 1D and 2D materials with different atomic coordinates will be introduced. Furthermore, a high-energy resolution EELS offers us possibilities to obtain local optical/vibrational properties. Some of the recent examples for such experiments on low-dimensional nanomaterials will be also presented [5-10].

References

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[11] The authors acknowledge funding from JST-CREST and ERC MORE-TEM projects.

Wednesday

09:45

Topological Engineering of Magnetism with Edge Defects in Graphene Nanoribbons

Steven G. Louie

UC Berkeley,
Department of Physics,
Berkeley CA, United States of America

Atomically thin quasi 1D and 2D materials exhibit fascinating phenomena, making their study one of the most exciting and rapidly advancing areas of materials research. In particular, defects in graphene nanostructures can induce novel magnetic behaviors in these π-bonded carbon materials. Employing topological classification theory and defect engineering, we have discovered a new class of graphene nanoribbons (GNRs), termed Janus GNRs (JGNRs). These JGNRs host diverse quantum magnetic phases – ranging from antiferromagnetism to ferrimagnetism to ferromagnetism – which can be tuned by controlling their defective edge structures, decorated with benzene-like motifs. In this talk, we will discuss their theoretical predictions and physical understanding. Our design principle and predicted properties for the JGNRs have been validated through bottom-up synthesis and scanning probe measurements.

This work was supported by the National Science Foundation.

Wednesday

10:25

Individual S vacancies and their role in anchoring of organic molecules on monolayers of MoS_2 on Au(111)

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Monolayers of MoS2 exhibit intriguing electronic properties, such as a direct band gap in the visible spectrum. This makes them particularly interesting for optoelectronic devices. When grown on a Au(111) surface, the electronic structures is strongly altered: Hybridization of the S states with the metal substrate leads to a reduced semiconducting band gap as compared to a free-standing layer. Yet, the metal-semiconductor structure still bears great potential for tuning molecular adsorbate structures.

Here, we introduce S vacancies into the top layer of MoS2 on Au(111). These exhibit a Kondo resonance at the Fermi level reflecting the presence of an unpaired electron spin [1]. We then deposit the thiol-based molecule CF3-3P-SH (tri-fluoro-methyl-*p*-terphenyl-thiol) on the defect-rich surface. Many of these molecules attach to the S vacancies. We find two categories of anchored molecules, those with and without a Kondo resonance. Density-functional theory calculations reveal that singly-occupied defects states persist when a dehydrogenated molecule is attached, while the hydrogen-terminated ones lead to doubly occupied defect states. These results explain the presence/absence of a Kondo resonance in experiment [2].

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Wednesday

11:40

Light Emission and Excitation of Single Atomic Defects in 2D Semiconductors

Laric Bobzien[1], Lysander Huberich[1], Jonas Allerbeck[1], Eve Ammerman[1], Nils Krane[1], Andres Ortega-Guerrero[1], Carlo A. Pignedoli[1], Oliver Gröning[1], Joshua A. Robinson[2], Bruno Schuler[1]

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Two-dimensional (2D) semiconductors provide an exciting platform to engineer atomic quantum systems in a robust, yet tunable solid-state system. This talk explores the intriguing physics of single point defects in transition metal dichalcogenide (TMD) monolayers, investigated through atomically resolved scanning probe microscopy.

We have determined the layer-dependent charge transfer lifetimes of selenium vacancies in WSe_2 on graphene substrates, spanning picosecond to nanosecond timescales [1]. By leveraging our recently developed lightwave-driven scanning tunneling microscope (THz-STM) [2,3], we could probe the ultrafast charge dynamics on the atomic scale. Time-domain sampling with a THz pump-THz probe scheme enabled capturing atomic-scale snapshots of transient Coulomb blockade, a hallmark of charge transport mediated by quantized defect states [4].

Moreover, the extended charge state lifetimes provided by hBN decoupling layers facilitated the local, electrical stimulation of excitonic emission from pristine MoS_2 and individual charged defects via STM luminescence (STML) [5].

By combining the structural and electronic properties accessible by conventional scanning probe microscopy with the optical fingerprint from STML and the excited-state dynamics revealed through pump-probe THz-STM, we gain a comprehensive microscopic understanding of localized quantum states in low-dimensional materials.

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Wednesday

12:20

Optical Properties of Defects in 2D Materials

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Defects in two-dimensional (2D) semiconductors play an important role for their potential applications in optoelectronic devices. Yet, for understanding the relation between the structure of the defects and their effects on the materials' electronic and optical properties, direct correlation between local, atomic-scale methods with optical spectroscopy is needed.

In this talk, I will present some recent results on intentionally and unintentionally introduced defects in 2D semiconductors investigated by correlative microscopy [1-3]. In monolayer and bilayer transition- metal dichalcogenides (TMDCs) we induce point-like defects by electron or ion irradiation and investigate them by photoluminescence (PL) and Raman spectroscopy. These measurements are combined with high-resolution electron microscopy at the same location of the sample. Furthermore, we discuss modifications of the 2D materials' properties by covalent functionalization.

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Thursday

09:05

Structure, Chemistry and Electrostatic Potential in Defective TMDs Probed by 4D-STEM

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Structural defects are known as a parameter-tuning knob for material properties. In particular, two-dimensional (2D) materials, with their unique infinitely large basal planes and atomic thickness, exhibit a vast range of atomic defects that present unparalleled degrees of freedom for tailoring physical properties. The ability to engineer atomic defects at the nanometer scale opens up unique opportunities to modify and enhance electrical, optical, mechanical, and magnetic properties. On the contrary, inevitable intrinsic growth-related defects appearing in synthesized materials such as grain boundaries (GBs) modify local electronic properties in a complex way, causing a discrepancy between the properties measured in synthesized materials and those theoretically predicted from a perfect model system. Identifying atomic defects and correlating their structural and chemical configurations with local electronic properties are therefore essential for synthesizing complex materials with desired characteristics and exploring their functionalities. Aberration Corrected Transmission Electron Microscopy (AC-TEM) has become the most powerful technique for providing detailed local atomic structure of 2D layers such as graphene and transition metal dichalcogenides (TMDs). Recently a new STEM acquisition technique so-called four-dimensional STEM (4D-STEM) has demonstrated its great potential to fulfil information either on up-scaled structures or on local electric states [1]. The technique consists in recording a diffraction pattern for each scanning beam position on the sample, enabling to visualize multiple structural information in micrometer scale. Analyzing the deviation of the transmitted beam position (Center of Mass: CoM) in 4D-datasets also gives access to the local electric field at atomic scale, and to the electrostatic potential and the charge density through Poisson's equation [2].

In this talk, the application of 4D-STEM for studying various defects in TMDs will be presented. Mapping domain junction in mono and multilayer films will illustrate the multi-scale analysis providing insight into the density and distribution of key atomic defects and the correlation between structure and property [3-4]. Atomic scale CoM imaging highlights the capability of 4D-STEM to probe negative charge accumulation around single dopant atoms in MBE grown WSe_2 monolayer. The electrostatic potential landscape in realistic structural configurations reveals the charge state of dopant atoms strongly influenced by other defects in their environments [5].

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Thursday

09:45

Atomically-precise Tailored Structures within 2D Materials

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Transmission electron microscopy (TEM) is often carried out separate from other experimental steps, allowing only “post mortem” analysis. This is a significant disadvantage compared to for example scanning tunneling microscopy, where the microscopic investigation is directly integrated as a part of the same experimental setup where the samples are grown and manipulated. There is however no fundamental reason why TEM and scanning TEM (STEM) could not be similarly integrated into more comprehensive system. In this overview presentation, I will present the experimental setup that we have established at the University of Vienna over the past decade to overcome this disadvantage [1]. I will further show how this setup and other advances made in the group in manipulation of 2D materials have enabled research towards truly atomically precise structures that can be tailored into 2D materials (e.g., Refs. [2-8]) for applications ranging from catalysis to quantum information technology. I will also briefly introduce the Vienna Microscope for Quantum Materials that is expected to be installed by the end of the year as an upgrade to the current Nion UltraSTEM 100 microscope.

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Thursday

10:25

Tip-enhanced Raman Spectroscopy of two-dimensional systems

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In this talk the use of nano-Raman spectroscopy to study two-dimensional (2D) materials will be discussed. Field coherence [1-7] and field distribution [8,9] are novel aspects that must be considered when addressing 2D systems in the nano (tip-enhanced) Raman spectroscopy (TERS) regime [10]. Our state-of-the-art results in graphene and transition metal dichalcogenides will be presented, exploring the connection between micro- and nano-Raman metrology [5,11]. Various aspects such as defects, homojunctions, twisted-bilayer structures, localized emissions at bubbles, wrinkles, and borders, as well as substrate effects will be considered. I will conclude by outlining some perspectives for nano-Raman spectroscopy in 2D systems.

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Thursday

11:40

Defect Mediated Growth of 2D Metallenes

W. Joudi [2], S. Ghaderzadeh [3], A. Trentino [2], K. Mizohata [1], G. Zagler [2], M. Längle [2], J. Madsen [2], C. Mangler [2], K. Mustonen [2], T. Susi [2], E. Besley [3], J. Kotakoski [2], E. H. Åhlgren [1,2]

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Defects in 2D membranes can be harnessed for the synthesis of new materials. They provide a chemical and structural framework that unlock the access to otherwise unfavorable and unattainable structures. In this work, we show how the normally inert basal plane of pristine graphene is functionalized by ion irradiation at the ultra-low energies in the range of few tens of eV's. The vacancy type defects that are introduced are then employed as anchoring sites to support the synthesis of various metal nanostructures on top and within the membrane. The structures are controlled by the specific conditions in which the metals are introduced and processed afterwards.

Individually dispersed metal atoms can be embedded within the graphene vacancies[1] providing an excellent platform for single atom catalysis. On the other hand, using thermal evaporation to introduce the metals, size selective nanoclusters can be grown[2], anchored to the dispersed embedded metal atoms. With a low ion beam current, a precisely controlled fluence and energy achieved by decelerating a beam of ions in a conventional 500kV air insulated ion implanter, 2D morphology can be achieved. This leads to the production of one-atom-thick metal[3] instead of the traditional 3D nanocluster.

The structures are imaged by means of high-resolution scanning transmission electron microscopy and the chemical composition is revealed by electron energy loss spectroscopy. Complementary atomistic simulations provide critical information on the role of the defects in the synthesis that can not be accessed with experiments. They reveal the energy landscape and elucidate the fs-timescale growth mechanisms. The presented results show that defects in

graphene offer a powerful tool to create controlled nanostructures for applications in single atom catalysis, energy conversion and optoelectronics.

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Thursday

12:20

Role of Defects in Oxidation of WS2 Surfaces and Interfaces

Katherine Milton, Daria Kieczka and Alexander Shluger

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The WS_2/SiO_2 interface is of interest to a variety of research communities due to the electronic properties of WS_2 and the ubiquity of SiO_2 as a dielectric substrate. Due to the hydrophilic nature of silanol groups on the surface of SiO_2, water is difficult to remove at the surface, leading to confined water between WS_2 and SiO_2. We investigated the structure and dynamics of confined water between WS_2 and SiO_2 using density functional theory and *ab initio* molecular dynamics, comparing it to adsorbed water on the surfaces of WS_2 and SiO_2 [1]. The results show that confined water becomes increasingly structured, with its orientation influenced by hydrogen bonding to the silanol groups as well as by the partial reorientation of water molecules to face WS_2 in an H-up configuration. The presence of silanol groups disrupts the hydrogen bonding network of water at monolayer coverage for both confined and unconfined water. For all interfaces explored, changes in both structural and dynamic properties are dependent on the number of water layers present. Using ab initio molecular dynamics simulations, we found that the confined water remains mobile but is structured by the interaction with WS_2 and SiO_2 with water protons drawn closer to both surfaces [2]. Although the presence of 1–3 water layers does not significantly affect the band alignment between SiO_2 and WS_2 and the electronic properties of the WS_2 monolayer, in-gap states caused by the dynamic rearrangement of water molecules can cause reduction of electron and hole mobility in the WS_2 layers. We find that on the pristine WS_2 surface, O_2 physisorbs in a triplet state, with a binding energy of 0.14 eV but may react with S vacancies and particularly vacancy clusters. Our DFT calculations [3] show that S vacancies will not migrate on the surface at the room temperature due to the migration barriers exceeding 2 eV. This suggests that vacancy clusters can form either as a result of sputtering or etching of the defective surface by oxygen. Reactions of O_2 molecules with S vacancy clusters are highly exothermic

and have small or no reaction barriers. However, the kinetics of the reactions of O_2 molecule with these clusters is complex due to several factors. Our *ab initio* molecular dynamics simulations demonstrate that O_2 molecules are highly mobile on the surface and easily desorb at room temperature due to weak interaction. Therefore, cross-sections for reactions with vacancy dimers and trimers, which require overcoming a barrier, can be small. We demonstrate that the reaction barrier depends on the S coordination of surface W atoms manifested in their effective charges – W atoms surrounded by three and more S vacancies have lower charges and are more chemically active. The O_2 dissociation on such sites proceeds without a barrier.

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Thursday

14:30

Modifications of Transition Metal Dichalcogenides by Incorporation of Excess Transition Metals

Matthias Batzill

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Reacting 2D materials with transition metals can result in compositional and structural rearrengments forming local defects or extended new materials. This provides a pathway for modifiying 2D sheets and transforming them into (meta)stable materials. Here the potential for such surface reactions, which may be characterized as 2D topotactical reactions, is discussd on the example of 2D transition metal dichalcogenides (TMDs). Three distinct examples are chosen to illustrate the breadth of the applicability of this approach: (i) the transformation of $PtTe_2$ into Pt_2Te_2 by reaction with Pt atoms (Figure (a) (see printed version)) [1] ; (ii) the reaction of Cr or Mn with bilayer VSe_2 to form VSe_2/Mn(Cr)/VSe_2 (Figure (b) (see printed version)) [2] and (iii) reaction of $MoTe_2$ with Mo to create mirror twin grain boundaries that may self-organize in periodic lattice networks (Figure (c) (see printed version)) [3,4]. The common concept in these surface reactions is that the reacted metals occupy ad- or absorption sites which maintain a low energy van der Waals termination and thus enables the creation of new (meta) stable 2D materials. The three examples discussed here illustrate the diversity of possible reaction products and the potential for synthesizing novel 2D materials by topotaxy.

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Thursday

15:10

Screening of material defects using universal machine-learning interatomic potentials

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Finding new materials with previously unknown atomic structure or materials with optimal set of properties for a specific application greatly benefits from computational modeling. Recently, such screening has been dramatically accelerated by the invent of universal machine-learning interatomic potentials that offer first-principles accuracy at a fraction of the computational cost. Their application to the screening of defects with desired properties or to finding new stable compounds with high density of defects, however, has not been explored.

In my presentation, I will describe our work on benchmarking leading universal machine-learning interatomic potentials for the screening of material defects, combining results from several existing defect databases [1]. We show that the universal machine-learning interatomic potentials have reached sufficient accuracy to enable large-scale screening of defective materials. We carried out vacancy calculations for 86 259 materials in the Materials Project database and analyzed the formation energies in terms of oxidation numbers. We further demonstrate the application of these models for finding new materials at/below the convex hull of known materials and for simulated etching of low-dimensional materials.

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Thursday

16:20

Creation and Characterization of Nanopores in Hexagonal Boron Nitride via Aberration-Corrected Scanning Transmission Electron Microscopy

Rachael Keneipp[1], Pia Bhatia[1], Jordan Gusdorff[2,3], Lee Bassett[3], Marija Drndic[1]

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The discovery of room-temperature single photon emission (SPE) in hexagonal boron nitride (hBN) launched it to the forefront of research as a promising platform for room-temperature quantum optics and photonics. Room-temperature quantum emission centers in hBN exhibit single-photon emission and optically addressable spin states, as desired for many quantum technologies. In this work, we create and characterize nanopores in hexagonal boron nitride (hBN) via aberration corrected scanning transmission electron microscopy (AC-STEM) drilling and photoluminescent (PL) spectroscopy. Using a finely tuned electron beam, defects on the sub-nanometer to nanometer scale are induced in hBN through electron irradiation and AC-STEM drilling. Atomic-resolution electron energy loss spectroscopy (EELS) is used to monitor and characterize the generation of these defects in real time, and atomic AC-STEM imaging is used to understand the atomic structure of the defects. Confocal PL spectroscopy is subsequently employed to characterize the optical activity of the defects created through electron irradiation and drilling. Through this work, we demonstrate the proof of principle to create defects in hBN of desired size, shape, and location. This work paves the way for controllable defect engineering in hBN and other 2D materials through AC-STEM drilling.

Thursday

17:00

Computer Modelling of Dislocations in Layered Materials

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Dislocations are a central concept in materials science, which dictate the plastic deformation, damage evolution and growth in materials. Layered materials such as graphite admit two general types of interlayer edge dislocation: basal and prismatic dislocations, of which prismatic dislocations have been relatively less studied I will present here our recent collaborative work on both edge and screw dislocations in graphite.

Screw dislocations in graphite were first reported by optical surface studies in 1952 [1]. Recent graphitisation studies have shown that screws are particularly stable and remain the primary structural defect after graphitisation of pyrolitic carbons at temperatures ranging up to 3500 K [2]. The fundamental Burgers vector along [0001] of 3.35 Å has been detected for recrystallised pyrolytic graphite [3]. Such a Burger's vector corresponds to a single interlayer distance and is demonstrated in a perfect dislocation in AA stacked graphite. Given the energetic instability of this stacking regime, it is unclear *a priori* how the dislocation structure contains itself within a predominantly AB-stacked graphitic environment. We investigate screw dislocation structure using the Atomic Cluster Expansion (ACE), a machine learning interatomic potential (MLIP) [4, 5]. This allows exploration of large-scale (many thousands of atoms) dipole structures with varying screw density. Furthermore, using a novel *registry stacking* method we have derived, we are able to provide a quantitative analysis of the local degree AA, AB, ABC or the intermediate stacking, taking into account the local curvature.

Using density functional theory (DFT) calculations, we have examined different prismatic core structures in graphite and evaluated their structure, energetics and mobility [6, 7]. We find close energetic interplay between bonded and "free-standing" core structures in both zigzag and armchair directions, with a reconstructed stable zigzag core identified. We explore grain

boundaries and prismatic dislocation pile-up, identifying metastable structures which may be important in energy storage. The role of interlayer stacking in core structure, dislocation glide and climb is also considered. Our calculations suggest that the prismatic dislocation core is stable up to high temperatures of approximately 1500 K in bulk graphite. Above this temperature, the breaking of bonds in the dislocation core can facilitate climb, grain-boundary motion, and the annealing of damage through prismatic dislocation glide. We also explore migration mechanisms for prismatic edge dislocations in graphite, including migration pathways along the c-axis direction and prismatic core interaction with point defects. The vacancy formation energy in the vicinity of edge dislocation cores is found to be substantially lowered, suggesting that mass-mediated motion of prismatic dislocations is limited at low temperature, where deformation will be primarily elastic and confined to basal planes. Implications for radiation damage, dimensional change, heat capacity, and melting are discussed. The existence of metastable magnetic dislocation cores, with significant transition barriers for non-magnetic reconstruction suggests that prismatic dislocations could account for much of the observed, weak ferromagnetic properties of irradiated graphite.

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Poster

#1

Room Temperature Gas Sensing with Hierarchical Bi-doped Sb_2WO_6 Microspheres: Effect of Oxygen Vacancies

Zichen Zheng[1,2], Kewei Liu[1,3], Yiwen Zhou[1], Zicong Zhang[1], Yongbin Qin[1], Yifan Luo[1], Kaichun Xu[1], Liangchao Guo[1], Marc Debliquy[3], Carla Bittencourt[2], Chao Zhang[1],*

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Summary

The incorporation of bismuth significantly enhances the gas-sensing performance of the Sb_2WO_6 microspheres, with the 4% Bi-doped sensing active layer achieving a remarkable response value of 15 when exposed to 200 ppm of CO_2, outperforming the undoped Sb_2WO_6. EPR analysis indicated the highest concentration of paramagnetic vacancies for 4% Bi compared with 0, 2 and 6 at.%. Furthermore, the selectivity of the 4%Bi-Sb_2WO_6 sensor towards CO_2 gas was enhanced relative to the Sb_2WO_6 sensor. The fundamental mechanisms of gas sensing and the factors contributing to the improved CO_2 response of 4%Bi-Sb_2WO_6 microspheres were investigated using density functional theory (DFT). These sensors present a novel platform for the identification and monitoring of CO_2, applicable in environmental monitoring, industrial processes and agricultural management.

Keywords: Antimony tungstate, carbon dioxide, doping, room temperature, DFT analysis

Background

Antimony tungstate (Sb_2WO_6), an n-type semiconductor characterized by the Aurivillius structure, has been extensively investigated in the field of catalysis due to its favorable band

gap (~2.3 eV). Nonetheless, its application in gas sensing remains underexplored [1]. Chemical doping with high electronegativity elements is an efficient strategy for improving gas sensing properties through modifications in morphology, crystal structure, and carrier concentration [2]. Bismuth, with an electronegativity of 1.9, has been shown to facilitate electron transfer and enhance the conductivity of Sb_2WO_6. The substantial difference in ionic radii between Sb^{3+} (0.76 Å) and Bi^{3+} (1.03 Å) likely induces lattice distortion, resulting in numerous crystal defects that improve gas sensing performance [3]. For example, Ma et al. reported the use of 0.75 mol% Bi-doped SnO_2 for NO_2 detection, achieving a detection limit of 50 ppb limit at 75 °C [4]. Zhang et al. demonstrated that Bi doping in Zn_2SnO_4/SnO_2 porous nanospheres sensors resulted in enhanced sensitivity, selectivity, and long-term stability to formaldehyde detection. Additionally, Cai et al indicated that Bi doping improves ethanol sensing performance [5]. In this study, hierarchical Sb_2WO_6 microspheres synthesized with an optimal Bi^{3+} doping amount, achieving a favorable combination of high response value (15 at 200 ppm), short response time (36 s at 200 ppm), good selectivity, and enhanced repeatability (200 ppm in 60 cycles) and long-term stability (4 repetitive cycles per day) at RT. DFT calculations indicate that the enhanced sensing properties of the Bi-doped Sb_2WO_6 arise from the tuning effects of Bi^{3+} substituting Sb^{3+} at adjacent W sites, thereby facilitating CO_2 binding.

Description of the New Method or System

A facile one-step hydrothermal approach was used to synthesize Bi-doped Sb_2WO_6. The resultant samples, corresponding to the varying amount of $BiCl_3$ added to obtain solution A: 0 mmol, 0.32 mmol, 0.64 mmol, and 0.96 mmol, were named Sb_2WO_6, 2%Bi-Sb_2WO_6, 4%Bi-Sb_2WO_6, and 6%Bi-Sb_2WO_6, respectively. The sensing layers were coated onto an alumina substrate (6*30 mm) with Pt electrodes by a droplet coating method. The gas-sensing test was performed via a four-channel gas sensing testing instrument, which measures electrical resistance signals of the corresponding channel in highly pure air and target gas. All the experiments conducted in dry air were at RT.

Results

The EDX mapping images demonstrate the presence of Sb, W, O, and Bi elements, confirming the uniform dispersion of Bi dopants throughout the material (Fig.1a) (see printed version).

To investigate the increase in defects generated during the solvothermal process, EPR analysis was conducted to characterize the unpaired electrons in Sb2WO6, as displayed in Fig. 1b (see printed version). The analysis revealed strong isotropic signals near g=2.003, consistent with

the g value associated with electrons trapped by oxygen vacancies. The sharpest signal of 4%Bi-Sb2WO6 indicates the highest concentration of paramagnetic vacancies concentration.

The transient response and recovery behaviors of all samples were assessed, as illustrated in Fig.1c (see printed version). Notably, the 4%Bi-Sb_2WO_6-based sensor exhibited a superior response across the entire detection range, suggesting that the optimum doping ratio of Bi^{3+} is 4 mol%. The enhancement in sensing performance can be attributed to the introduction of Bi atoms as donor sites, resulting in maximum response to 1000 ppm CO_2 that is six times greater than that of pristine Sb_2WO_6. However, a decrease in performance was observed when the Bi doping level exceeded 4 mol%, primarily due to the saturation of surface sites and disruption of the structure, which reduced the interaction probability between CO_2 and the sensing layer.

The 4%Bi-Sb_2WO_6-based sensor also demonstrated a rapid response time (~36 s), which is essential for real-time detection (Fig. 1d) (see printed version).

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Poster

#2

Defect-engineering hexagonal boron nitride using low-energy Ar+ irradiation

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Hexagonal boron nitride (hBN), mostly known as an electrically insulating structural counterpart of graphene, has recently become the focus of intense research as a material to host quantum emitters [1]. Particularly their potential to host single photom emitters at room temperature opens up potential applications in quantum communication, information and simulation as well as photonics. Although such emission is well known to be associated with point defects, so far no conclusive correlation between the spectra and specific defects has been demonstrated, partly due to the challenge of controlling and characterizing their atomic structure. Therefore, it would be desirable to be able to selectively create specific types of point defects in hBN and to characterize their atomic structure over an optically relevant spatial extent.

Ion irradiation is a promising technique for the generation of defects in 2D materials due to its general applicability. Analytical potential molecular dynamics simulations of ion irradiating hBN [2, 3] have suggested that low-energy noble gas ions should lead to the formation of point defects with high likelihood (40 – 80% per ion) and similar probabilities for single boron and nitrogen vacancies. Especially according to simulations with an improved potential benchmarked against density functional theory (DFT), the best selectivity should be achievable at the lowest energies (<200 eV), where nitrogen single vacancies become clearly more favorable for projectiles heavier than Ne [3].

Here, we prepare atomically clean suspended hBN samples and subject them to low energy Ar + ion irradiation (20 – 200 eV) [4]. The samples are characterized before and after irradiation via atomic-resolution scanning transmission electron microscopy imaging to assess the defect concentrations and distributions. Statistically significant amounts of data are recorded via semi-automated image acquisition and analyzed via convolutional neural network [5]. The defect concentration before and after irradiation for one energy are shown in the figure below (see printed version). The most commonly found defect is the boron single vacancy in contrast to the prediction from molecular dynamics, followed by nitrogen single vacancies, double vacancies and more complex structures.

The first main challenge in this work is the combination of acquiring atomic-level understanding with sufficient statistics. This requires keeping the sample atomically clean, so avoiding exposure to air. This means we can not use specialized ion-irradiation set-ups but have to use a plasma source within the ultra high vacuum system directly connected to our microscope. This is particularly important with irradiated samples as defects notoriously attract contamination which then prevents us from imaging the introduced defects. The second main challenge is the beam-sensitivity of hBN, requiring fast imaging to minimize the beam induced defects, while at the same time hBN is one of the most difficult specimen to image in STEM due to the low atomic numbers of boron and nitrogen. The third challenge is sample preparation with sufficient quality. As is shown in figure (see printed version) one already the non-irradiated samples show a significant number of defects.

Overall, the results so far demonstrate that the simplest irradiation already provides selectivity for the defect types. This opens the challenge towards optimizing the irradiation parameters (species, energy or angle) for also selectively creating other defects. With this we will provide a significant contribution towards understanding defect creation via low-energy ion irradiation at the atomic level. After this we hope to be able to correlate the created defects to the specific single photon emission properties of the material and thus open up the way towards true understanding of emission properties of hBN.

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Poster

#3

Defect Engineering in MoS_2 Nanomaterials via Low-Energy Ion Implantation for Next-Generation 2D Functional Devices

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The exploration of two-dimensional (2D) materials, such as molybdenum disulfide (MoS_2) and other transition metal dichalcogenides (TMDs), has gained significant attention due to their extraordinary electronic, optical, and mechanical properties. These materials hold immense potential for applications in electronics, optoelectronics, catalysis, and energy storage [1,2].

Ion implantation has emerged as a promising technique for modifying the structure and properties of 2D materials by introducing dopants and defects into the atomic lattice, as shown in Figure 1 (see printed version). This process enables precise control by creating desired configurations such as substitutional dopants, vacancies, and interstitials while minimizing unwanted defects, opening a way to modify the material's electronic, optical, and mechanical characteristics. This research explores how low-energy ion implantation can modify MoS_2 atomic structure and properties, unlocking applications in catalysis, optoelectronics, and other advanced fields [2,3].

Existing research primarily focuses on the effects of high-energy ions on 2D materials. In contrast, the impact of ultra-low-energy ions, such as argon (Ar) and xenon (Xe), on MoS_2 has not been as thoroughly investigated. This research aims to fill this gap by studying the effects of ultra- low-energy ion implantation on MoS_2 at varying ion energies by experimental and computational approaches. Additionally, scanning transmission electron microscopy (STEM) analysis and Raman spectroscopy are used to perform detailed structural characterization. Molecular Dynamics (MD) simulations will help create predictions and understand

experimental results. By combining these approaches, this research aims to deepen the understanding of how ultra-low-energy ion implantation influences the properties of MoS_2.

Employing the KIIA ion accelerator at the University of Helsinki, mechanically exfoliated MoS_2 samples were irradiated at controlled doses (1×10^{14} – 1×10^{15} ions/cm^2) and energies ranging from 15 eV to 200 eV. STEM analysis revealed significant structural alterations, including defect formation at energies 40, 45, 50, 55, 80, and 200 eV. A clear indication of trapping the ions in the van der Waals gap is seen in the simulation at 40, 45, 50, and 55 eV, but the experimental confirmation is still underway. The transition from AB stacking to mixed AB/AA/AC stacking was observed, with stacking transformations occurring at the sub-nanometer scale shown in Figure 2 (d) (see printed version).

To complement the experimental findings, extensive MD simulations were conducted using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) to study the atomic-scale interactions of low-energy Ar and Xe ions with the MoS_2 lattice. The simulations employed the REBO (Reactive Empirical Bond-Order) potential for Mo-S interactions due to its accuracy in capturing bond breaking and formation. The Ziegler–Biersack–Littmark (ZBL) potential was used to model ion-lattice interactions, ensuring an accurate description of collision dynamics [4]. The results illustrated in Figure 2 (e)-(h) (see printed version) revealed that at 20 and 30 eV, no defects were introduced, while a threshold of 35–40 eV initiated defect generation in the top MoS_2 layer. At 40–50 eV, Ar ions penetrated the first MoS_2 layer, leading to interlayer trapping, nanoscale pore formation, and stacking disorder.

The sputtering yield of Mo and S was analyzed as a function of ion energy, revealing that sulfur atoms were preferentially sputtered at lower energies due to their lower binding energy compared to molybdenum [5]. At higher doses, preferential S depletion led to Mo-rich defect configurations. Additionally, Ar ions exhibited interaction pathways, some trapped within the van der Waals gaps and others backscattered, depending on their incident energy. In contrast, due to their higher mass compared to Mo and S, Xe ions induced pore formation at a lower energy threshold, making them more efficient for defect engineering applications where porosity is required.

A key innovation of this study is the demonstration that 15 eV Ar implantation achieves clean surfaces and well-preserved MoS_2 surfaces, presenting a promising method for surface cleaning when applied prior to precise property engineering. Our findings establish a precise

energy window for controlled defect introduction in MoS_2, allowing for tailored modifications suitable for nanoelectronics, optoelectronic, and catalytic applications.

This study provides critical insights into how ultra-low-energy ion implantation can be employed as a precise tool for defect engineering in MoS_2, uncovering the mechanisms of dopant incorporation, defect formation, and structural evolution to fine-tune its properties for specific applications. However, challenges remain in achieving precise control over ion implantation to introduce desired defects and dopants without causing excessive damage that may negatively impact the material properties. Future work will focus on refining implantation techniques, optimizing defect configurations, and assessing their properties, further expanding MoS_2's applicability in nanoelectronics and sustainable energy solutions.

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Poster

#4

Spectrally resolved far-field emission pattern of single sulfur vacancies acting as single photon emitters in MoS_2

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We explore the optical dipole orientation of spatially positioned single photon emitters in monolayer MoS_2 as produced by a focused helium ion beam [1,2]. The single photon emitters can be understood as single-sulfur vacancies [3]. The corresponding far-field luminescence spectra reveal several photoluminescence lines below the dominating luminescence of the defect-related exciton in MoS_2. These sub-bandgap emission lines were predicted by ab initio theory [4], but they have never been resolved in luminescence experiments because of their small amplitude. We reveal the lines by their dependence as a function of the photon energy and momentum as measured in the back focal plane of the optical circuitry (cf. Figure 1 (see printed version)). The agreement between our ab-initio calculation based on many-body perturbation theory within the GW and Bethe Salpeter equation (GW-BSE) approach and the demonstrated experiments suggests that the defect states interact strongly within the Brillouin zone of the investigated crystals [5].

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Poster

#5

Revealing the atomistic structure of carbon nanomembranes: molecular dynamics simulations and experiments with highly charged ions

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Carbon nanomembranes (CNMs) are a new class of near-2D membranes with potential applications ranging from energy storage and generation, through to water filtration. It has recently been shown that highly-charged ions can be used to introduce additional nanoscale pores to these membranes, where the pore diameters can be controlled by varying the kinetic and potential energy (incident charge state) of the impinging ions [1,2]. Additionally, when these transmitted ions interact with CNM, or indeed any thin material, they carry with them information about the original structure which can then be extracted by interrogating the resultant distribution of final ion charge states [3]. Here, we use a coupled experimental and simulation approach to identify candidate atomistic structures of a typical CNM, from those generated via liquid-quench and annealing molecular dynamics simulations. Experimental and simulated ion charge exchange data suggest that CNMs have an innate sub-nanometer porous structure. Furthermore, these membranes may have an under-coordinated carbon network that would be stabilised when exposed to atmospheric conditions. The candidate CNM structures identified will also be valuable for future computational studies, e.g. elucidating the mechanism of water and gas permeation. Our results shed new light on the atomistic structure of CNMs.

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Poster

#6

Atomic manipulation approach towards defect engineering in two-dimensional materials

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Low dimensionality, inherent to the class of two-dimensional (2D) materials, allows for the existence of a large variety of many-body phases. While these phases are interesting on their own, they also present an excellent platform for the creation of novel exotic states using atomic defects such as adatoms and vacancies. An additional advantage of 2D materials as hosts for quantum defects is, that they are easily accessible for scanning probe measurements like scanning tunneling microscopy.

An especially fruitful field is the exploration of point defects in two-dimensional semiconductors like MoS_2 or WS_2 [1]. Here, the presence of point defects can lead to the formation of well isolated in-gap states that could have potential applications in quantum information technology [2]. However, so far, these investigations focused on point defects that were introduced to their host during growth or post-growth via annealing or ion beam bombardment. Control over their exact location with respect to the atomic lattice remains elusive, hampering the creation of extended artificial defect structures.

One approach envisioned to allow for local defect engineering with atomic-scale precision is atomic manipulation using a scanning tunneling microscope. Here, single atoms can serve as building blocks for the construction of novel and exotic point defects. These atoms can either be adsorbed onto or incorporated into the 2D material of interest and arranged in a custom

way. While atomic manipulation experiments with (magnetic) adatoms on bulk crystals have successfully been performed in the past [3], reports for manipulation on 2D materials are very limited [4] and the creation of well-defined defect structures within 2D materials by atomic manipulation has not been achieved to the best of our knowledge.

In this work, we perform atomic manipulation experiments to engineer point defects in 2D materials. Two different systems are compared to each other: Fe on 1H-MoS_2 and Fe on 1H-TaS_2. We find that manipulation of single Fe atoms on the semiconductor 1H-MoS_2 results in the creation of sulfur vacancies, which we investigate using scanning tunneling microscopy and spectroscopy [5]. Our investigations reveal the existence of two symmetry-broken states in negatively charged vacancies, which we realize through local tip gating and which can be attributed to Jahn-Teller distortions. Additionally, we discuss hybridization effects in dimers of sulfur vacancies and the potential of larger artificial vacancy structures for tailoring custom in-gap states.

In contrast, we find that single Fe atoms can be laterally manipulated on metallic 1H-TaS_2 without changing the atomic structure of the 2D material. Here, the Fe atoms adsorb on two inequivalent sites, metal-centered (MC) and hollow-centered (HC) sites, which manifests as differences in the adatom's apparent height. This paves the way for the construction of extended adatom lattices which could be a promising platform for customizable magnetic states on 2D materials.

The fact that the two systems under investigation show markedly different behavior might serve as a motivation to extend this study to other 2D materials, to enable a comprehensive understanding on the interactions between adatoms and 2D materials. These interactions not only involve the binding energy of adatoms and therefore the manipulation capabilities, but will also influence the ground state of the system.

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Poster

#7

Nanoscale Engineering of Defects in Hexagonal Boron Nitride with an Electron Beam and its Applications from Quantum Technology to Nanofluidics

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The ability to precisely engineer atomic-scale defects and nanopores in two-dimensional (2D) materials is of increasing demand due to the unique properties and applications these defects afford 2D material systems. Recently, the 2D material hexagonal boron nitride (hBN)—and its defects—have become of interest across numerous fields because of the exciting properties and applications the defects in hBN introduce. The discovery of room-temperature single-photon emission [1] in hBN thrust it to the forefront of quantum technology research as a host for single-photon sources and spin qubits, and the high surface charge of hBN [2] makes it an exciting platform for high ion selectivity in nanoporous systems. Sub- nanometer defects and nanopores in 2D materials, including hBN, are ideal candidates for biomolecule sequencing [3], osmotic energy generation [2], and water filtration [4]. However, methods for controllably engineering materials at the sub-nanometer scale are lacking, especially in multilayer 2D materials.

In this work, we report the ability and methodology of engineering features in multilayer hBN of thickness ~ 5 to 20 nm down to the sub-nanometer scale. We demonstrate the use of electron energy loss spectroscopy (EELS) as a tool to monitor the progress of aberration-corrected scanning transmission electron microscopy (AC-STEM) thinning and drilling (Figure 1a (see printed version)). EELS is used to monitor the drilling progress and atomic composition of B and N through relative signal strength. Such use of EELS allows us to also detect drift while drilling and to monitor the relative remaining thickness of the hBN, affording the capability to finely monitor drilling progress layer-by-layer [5]. We demonstrate this technique at different beam energies (80 keV, 200 keV) and experimentally determine how the use of these varied electron beam energies leads to differences in drilling time, pore shape, and other defects induced in the material. At each beam energy, EELS data is collected throughout pore drilling with the drilling time. We also demonstrate the ability to controllably thin complex sub-nanometer shapes and features in hBN at 200 keV as shown in Figure 1b (see printed version). Through e-beam etched patterns and defects, we show with atomic- resolution AC-STEM imaging the effects of varying drilling times on the defect size and hBN structure.

Furthermore, we investigate the properties of these defects and their promise for applications in quantum technology and nanofluidics. In this work, the effect of AC-STEM defect engineering on the local optical activity of multilayer hBN towards deterministically creating quantum emitters in hBN was investigated. Patterns were etched in hBN via EELS-monitored AC-STEM drilling with an 80 keV electron beam and were correlated with subsequent photoluminescence (PL) measurements. Figure 1c (see printed version) shows how AC-STEM drilling of hBN was used to controllably induce local optical activity in electron- irradiated regions. We did not observe evidence for single-photon emission in these regions, and the enhanced PL features appear to be spatially extended beyond the optical diffraction limit, suggesting that the beam exposure affects optical activity on the scale of several hundred nanometers. Nonetheless, the clear correlation of optical changes with the e-beam irradiated regions presents opportunities for future studies to explore the exact relationship between the atomic structure of electron-beam-induced defects in hBN and the resulting photoluminescence. AC-STEM drilling was also used to engineer sub-nanometer pores for nanofluidic applications. Current-voltage (I-V) characteristics were obtained for nanometer and sub-nanometer hBN pores with different pore sizes. Figure 1d (see printed version) shows two pores with diameters of ~ 1.2 nm (blue outline) and ~ 0.8 nm (red outline) and the resulting I-V curves taken from the two pores in 1M KCl. The collected I-V curves were linear I-V

with finite values of ionic current, suggests that the nanopores are open and wetted. Such pores could be used for sensing of very small biomolecules, such as peptides or hormones, or for osmotic energy generation. Overall, our work opens new doors for the fields of correlated measurements, nanofluidics and nanosensing.

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Poster

#8

Nanostructuring of 2D materials using slow highly charged ions

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The ability to precisely tailor 2D materials and heterostructures thereof is crucial for their integration into next-generation nanodevices. In this work, we focus on highly charged ion (HCI)-induced nanostructuring, a technique capable of perforating 2D materials with monolayer precision [1]. HCIs store large amounts potential energy, which equals the sum of binding energies of all removed electrons, e.g. about 40 keV in the case of a 40-times charged Xe ion. Upon approaching a sample surface, this potential energy is released within the very first layers of the material, where the depth of energy deposition can be tuned via the incident ion charge state and kinetic energy [2]. In 2D materials and heterostructures, this can be employed to tune pores of a certain size.

R. Kozubek *et al.* [3], for instance, demonstrated charge-state-dependent nanopore formation in free-standing monolayers of MoS_2, with increasing ion charge states resulting in larger pore diameters on the order of 1–5 nm. In contrast, E. Gruber *et al.* [4] conducted similar experiments with graphene monolayers and observed no pore formation. These differing results highlight the importance of electronic properties of the irradiated materials: MoS_2, a semiconductor, dissipates electronic excitation differently than graphene, a semi-metal. Together, this can be applied to precisely tune hetero- structures of both materials shown recently by J. Schwestka *et al.* [1]. Depending on the orientation of the heterostructure (i.e. which material faces the ion beam first), MoS_2 was found to be perforated (with graphene

behind still intact, cf. Figure 1 (see printed version)) or shielded from being damaged (by a graphene layer in front).

Besides the empirical finding of different susceptibility of conducting and insulating surfaces to desorption by strong electronic excitations by HCI, the coupling between a highly excited electronic system on the nanoscale to lattice atomic motion remains still elusive. A. Grossek *et al.* [5] proposed a hopping model, leading to a phase diagram of the susceptibility of a material to HCI-induced nanostructuring depending on electronic material properties and ion charge state. However, so far these results could only be benchmarked with previous results in literature for semi-metal graphene [4] and semi-conducting MoS2 [3], respectively, and more experiments across a wider range of 2D materials with different properties will be necessary to refine predictive models and optimise nanostructuring techniques. Here, we present new data on pores induced in free-standing monolayers of insulating hexagonal boron nitride (hBN). Our results align with existing models [5], and provide new insights into how material properties influence nanostructuring.

However, even though our models yield good qualitative agreements with experiments, no quantitative or predictive modelling could yet be achieved for nanostructure formation by HCIs. Producing more experimental data for benchmarking theoretical predictions, hence, is critical for the future integration of HCI-based nanostructuring into scalable material processing methods, where they could be benefiting applications in nanoelectronics and filtration.

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Poster

#9

Correlated Structural and Optical Characterization of Hexagonal Boron Nitride

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Hexagonal boron nitride (hBN) is a van der Waals material uniquely poised to play a key role in quantum information science, given its bright quantum emission at room temperature. Some emitters display spin-dependent optical properties and can therefore be utilized as spin qubits.[1-3] However, these emitters are not yet fully understood. Moreover, identifying emitters in two-dimensional materials is especially complex because they are sensitive to interfaces and other local environmental effects (e.g., defects, strain, and contamination).[4-5] Therefore, understanding and controlling the properties of hBN, especially at its surface, will be crucial to advancing scalable quantum information and photonics technology.

While the optical properties and material structure of hBN are often studied separately, few studies have investigated them in parallel. Even fewer have utilized transmission electron microscopy (TEM) in parallel with photoluminescence (PL) microscopy to shed light on the structure of emitters in hBN. Therefore, we combine PL, TEM, white-light microscopy, energy dispersive x-ray spectroscopy (EDS), *and* atomic-force microscopy (AFM) to elucidate the relationship between optical properties and material structure in hBN. We study changes in optical activity and flake morphology associated with different sequences of measurements and treatments, focusing on overall statistical properties of the material, rather than few-atom defects or single emitters. Figure 1 (see printed version) summarizes our key observations from a ~28-nm-thick flake of hBN included in this study. The flake was mechanically exfoliated from bulk and transferred onto patterned silicon nitride membranes via polydimethylsiloxane (PDMS) viscoelastic stamping. Membranes were patterned with circular holes to suspend part of the hBN flake and mitigate substrate-induced effects in the suspended region. Figure 1(a)

(see printed version) depicts a cross-sectional schematic of our device geometry, and the specific sequence of measurements performed on this sample.

First, we observed that PL measurements themselves induce photobleaching in hBN (Fig. 1(b-c). We quantified this observation by performing a statistical analysis which classifies emitters based on density and brightness (Fig. 1(d)), *before and after* photobleaching. Next, this sample was subject to electron beam irradiation in the TEM. Imaging of a representative region of this flake (boxed in magenta in Fig. 1b)) was performed and revealed that the flake was covered with a homogeneous film of residue (Fig. 1(e)). Qualitatively, the residue appeared to clump together and diminish with increasing irradiation time (Fig. 1(f)), resulting in the lacey network of residue shown in Fig. 1(g). We quantitatively analyzed this residue and characterized its spatial distribution; the results of this analysis are shown in Fig. 1 (h-j). Interestingly, we observed that both the surface coverage and mean area of the residue increased slightly over the first 25 minutes of TEM exposure and then decreased after 40 minutes. Subsequent PL imaging (Fig. 1(k-m)) demonstrated a corresponding, non-monotonic change in emission. We also performed elemental dispersive x-ray spectroscopy (EDS) to better understand the chemical composition of the residue present on this hBN sample. EDS maps indicate that the residue is primarily comprised of silicon, oxygen and carbon species which are consistent with the PDMS viscoelastic stamping procedure used to transfer hBN flakes in this study (Fig. 1(n-p)).

In the sample shown in Figure 1 (see printed version) and across the other samples studied, *all* optical emission was unstable and subject to photobleaching. Similarly, electron beam irradiation resulted in morphological changes to flake residue, which was then correlated with changes in optical emission. Future work could utilize the correlative measurement procedure introduced here to examine a variety of parameters relevant to quantum emission in hBN. For example, correlative TEM and PL measurements could be used to systematically compare the effect of different transfer methods on the cleanliness and optical activity of hBN. Such work may shed light on the role of lattice substitutions on emission in hBN. Similarly, it may also be of interest to utilize this method to study how flake thickness mediates the cleanliness of transferred flakes (if at all) and their resulting optical activity. In short, a quantitative understanding and ability to reliably control surface contamination is essential to engineering *all* 2D materials. In this case of hBN, our hope is that this work represents a meaningful step towards a scalable means of generating and controlling single quantum emitters in hBN.

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Poster

#10

Controlled substitutional doping of MoS_2 for gas sensing applications

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Gas sensors play a crucial role in environmental monitoring, industrial safety, and healthcare applications. Traditional chemiresistive gas-sensing technologies, such as semiconductor metal oxide (SMO) sensors, rely on oxidation-reduction reactions that require high operating temperatures. This leads to significant power consumption and integration challenges with modern electronics, as microheaters are necessary for their operation. In contrast, 2D materials have emerged as highly promising candidates for gas sensing because their sensing mechanism is based on charge transfer between the sensing film and the adsorbate, which eliminates the need for additional thermal energy. Among these materials, monolayer MoS_2 stands out due to its intrinsic direct band-gap, making it a prime candidate for future gas-sensing devices; however, a major limitation of MoS_2 is the relative chemical inertness of its basal plane, which leads to low sensitivity, long response times and poor selectivity of pristine MoS_2-based gas-sensors.

To adress this limitation, the material must be modified to introduce more active adsorption sites. Substitutional doping with precious metals, such as Pt, is a particularly promising modification method of particular interest because it creates well-defined and practically isolated active sites, which not only helps to increase the sensitivity of the sensor, but also its selectivity and specificity.

Although substitution of sulfur atoms with Pt has been achieved using methods such as isolating single Pt atoms from clusters [1], Pt atom intercalation during chemical vapor deposition (CVD) [2] and hydrothermal growth [3], the exact placement of the dopants remains

ambiguous in many of these studies. This ambiguity often arises due to the lack of atomic-scale imaging or, in cases where such imaging is provided, the use of high-angle annular dark-field (HAADF) scanning transmission electron microscopy (STEM). The bright contrast of the heavy Pt atoms in HAADF obscures the surrounding atomic structure, making it difficult to differentiate between Pt atoms occupying a single or a double sulfur vacancy.

In a recent study [4] we overcome these limitations by employing single-sideband (SSB) ptychography, a technique that was previously demonstrated to successfully in differentiate vacancies in MoS_2 at atomic resolution [5]. We introduce defects into MoS_2 using low-energy helium plasma irradiation, followed by detailed analysis of the resulting defect structures. Subsequently, we evaporate Pt atoms onto the defect- engineered MoS_2, and observe the placement of the dopants by imaging the material after each step, combining HAADF and SSB imaging with image simulations. We emphasize that the combination of these techniques is crucial for accurate analysis, as both HAADF and SSB imaging have their limitations which could lead to false conclusions when used independently. We demonstrate that these imaging methods allow differentiation between Pt adatoms, Pt atoms implanted into the lattice, and even Pt atoms embedded in single versus double S vacancies (see figure (see printed version)). This distinction is particularly significant for gas sensing applications, as the atomic-scale placement of the dopants has a strong influence on the local electronic structure, which in turn governs the gas-adsorption properties, especially in regards to selectivity. Our substitutional doping process is not only scalable, but also trivially adaptable to other substitutional atoms and materials.

So far, we have successfully implanted Pt atoms into Mo- and S lattice sites at a large scale, but the con- trol of the implantation site is still limited by the inherent randomness of the defect creation process. To provide more control over this step we are currently experimenting with tuning the ion beam parameters and incorporating a resulfurization step to heal remaining sulfur vacancies. Even though we conduct the majority of our experimental steps within the boundaries of our unique fully integrated CANVAS ultra-high-vacuum system, surface contamination remains the most significant challenge. Contamina- tion not only shields parts of the pristine sample surface from ion irradiation but also covers already irradiated areas, preventing the incorporation of Pt atoms. To limit the influence of the contamination we explore additional cleaning in-between the fabrication steps using thermal or laser-annealing, but optimal parameters must be identified to allow for efficient contamination removal without damaging the relatively heat-sensitive material.

In future we will probe our modified Mos_2 samples using a custom designed gas sensing setup, that allows to probe micro-meter scaled devices irrespective of their layout or design. The sensing measurements will be supported by ab-initio device-simulations and DFT adsorption simulations that give us a deeper understanding of the charge transfer process between selected gasses and the engineered active sites.

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Poster

#11

2D Interfacial Modification in Dimethyl Sulfoxide (DMSO) Free Tin Halide Perovskite over 10% PCE

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Perovskites are a class of materials characterized by the crystal structure ABX_3 where A(methylammonium MA^+, cesium Cs^+ or formamidinium FA^+), B(lead Pb^{2+} or tin Sn^{2+}) and X(iodide I^-, bromide Br^- or chloride Cl^-)are emerging as promising candidates for next-generation photovoltaic and optoelectronic applications. Perovskite solar cells (PCSc) have emerged as a highly promising photovoltaic technology due to their cost effective fabrication processes and remarkable power conversion efficiencies. In 2009, PSCs were initially proposed as visible light sensitisers for photovoltaics, with 3.8% power conversion efficiency (PCE) at the laboratory scale to date, reaching an extraordinary 26.95 %. However, the environmental and health concerns are associated with Pb in high performing PCSs. Tin perovskite solar cells (Sn-PSCs) are considered as eco friendly alternatives to there Pb based PSCs. Ploy (3,4-ethylenedioxythiophene) polystyrene sulphonic acid (PEDOT.PSS) as hole transport layer (HTL) and dimethyl sulfoxide (DMSO) employed for Sn-PCSs approaching 16% but they are leading towards fast Sn oxidisations. Herein we interduce Phenethylammonium iodide (PEAI) in PEDOT.SS/DMSO free perovskite composition $FA_{0.95}EDAI_{0.05}SnI_3$ as 2D buried interface modification. Incorporation of 2D PEAI improves the morphology and crystallization of Sn-PSCs, trSPV result confirms the less charge recombination between HTL/PVK interface. As the result fabricated device first time achieved a remarkable PCE of 10.3% in DMSO free system under simulated AM 1.5G illumination.

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Poster

#12

Mycosynthesis of Silver nanoparticles for Energy Application

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The present study addresses an eco-friendly and energy-saving method for extracellular biosynthesis of silver nanoparticles (AgNPs) using a cell free filtrate of the fungus strain *Aspergillus niger* and *Fusarium semitectum* as a reducing agent. Parametric optimization of the biosynthesis process demonstrated different effects on the size, distribution, yield, and synthesis rate of biosynthesized AgNPs. SEM micrograph showed polydisperse spherical and ellipsoid nanoparticles (SIZE). X-ray diffraction (XRD) analyses indicated that AgNPs were nanocrystalline by nature, with the character of a face-centered cubic (fcc). Furthermore, the biosynthesized AgNPs exhibited higher antimicrobial activity than silver ions against *E.coli, Staphylococci, and Pseudomonas*. These results demonstrate that mycosynthesis of silver nanoparticles is a cost effective, eco-friendly way and its antibacterial properties also used in an as efficient antimicrobial agent.

Keywords: Silver nanoparticles; extracellular biosynthesis; *Aspergillus niger; Fusarium semitectum*; antimicrobial activity.

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Poster

#13

Defect-Induced Modulation of the Electronic and Magnetic Properties in CrSBr Monolayers

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The two-dimensional CrSBr compound and its van der Waals layered counterpart have aDracted considerable aDenEon due to their unique electronic and magneEc properEes [1,2]. However, the impact of defects on their characterisEcs remains poorly understood. Meanwhile, ion and electron irradiaEon have been experimentally demonstrated as effecEve tools for defect-mediated engineering of this material [3,4].

In this study, we employ first-principles calculaEons to gain insight into the energeEcs and properEes of point and line defects in CrSBr monolayer. We analyze defect formaEon under electron irradiaEon by evaluaEng atomic displacement thresholds and calculaEng displacement cross-secEons as funcEons of electron energy within the McKinley-Feshbach formalism. AddiEonally, we invesEgate the electronic and transport properEes of finite-width nanoribbons with armchair and zigzag edges. Our results reveal that the band gap of CrSBr nanoribbons depends on both their orientaEon and width, while the edges exhibit spin-polarized electronic states. These insights pave the way for defect-mediated engineering of CrSBr systems for spintronic applicaEons.

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